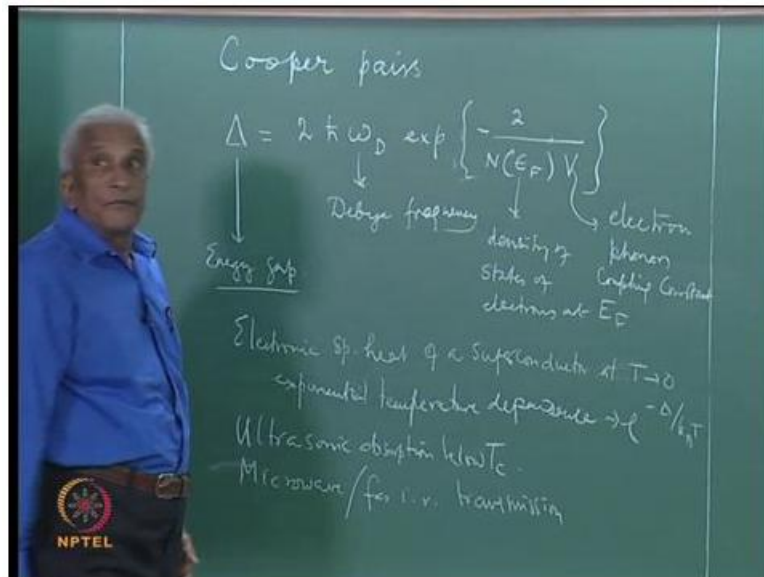


Condensed Matter Physics
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Lecture - 31
Microscopic (BSC) Theory of Superconductivity

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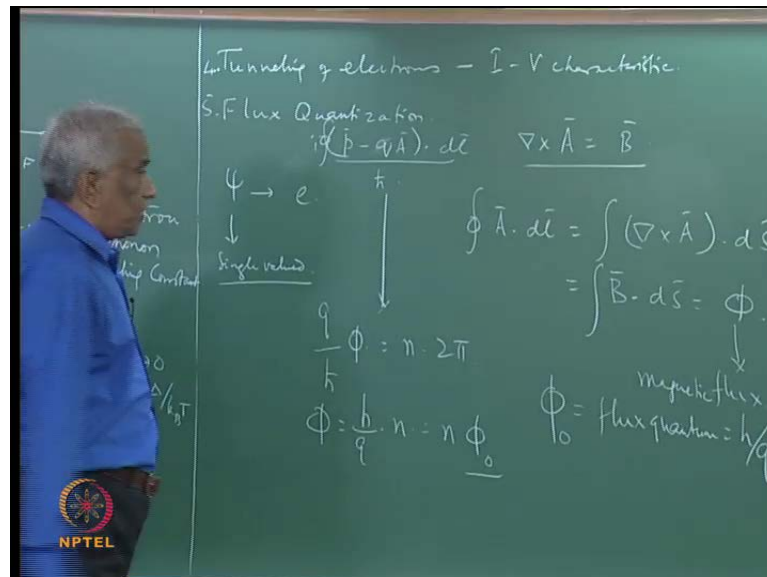
In the last lecture we discussed the quantum mechanical problem of founding a bound state for a pair of electrons, when there is a net weak attractive interaction between them, which is mediated for example, by the coupling of the electrons to phonons. This was a problem which was handled first by Cooper, and the electron pairs thus forming the bound state are known as Cooper pairs. And we saw that in the presence of one electron-phonon coupling, which brings about a net attractive interaction between the pair of electrons forming the Cooper pair. We get a net lowering of energy given by an amount where ω_D with Debye frequency, this is the density of states of electrons at the Fermi energy E_F in this is the electron-phonon coupling constant.

So, the energy of the bound pair is lower than that of the separated normal state electrons, and therefore energetically these are favorable to form Cooper pairs for these two electrons. Now, the existence of such a gap which opens at the Fermi level is experimentally supported by techniques, such as the specific heat of a superconductor at very low temperatures. So, this is an exponential temperature dependence very similar to what you find in a system such as a semiconductor we will discuss this shortly, where there is an energy gap. So, similarly the exponential

temperature dependence indicates an activation of the carriers responsible for thermal transport in this case. So, there are excited across this gap Δ and that is why there is an order to do that they have to have an activation energy of this order, so this goes as an exponential minus Δ by $k_B T$.

So, that is the temperature dependence which is observed you can determine the energy gap. The second experiment is that of ultrasonic absorption below T_c , and the third experiment is microwave or for infrared transmission in superconducting films. So, these are experimental evidences for the existence of the energy gap.

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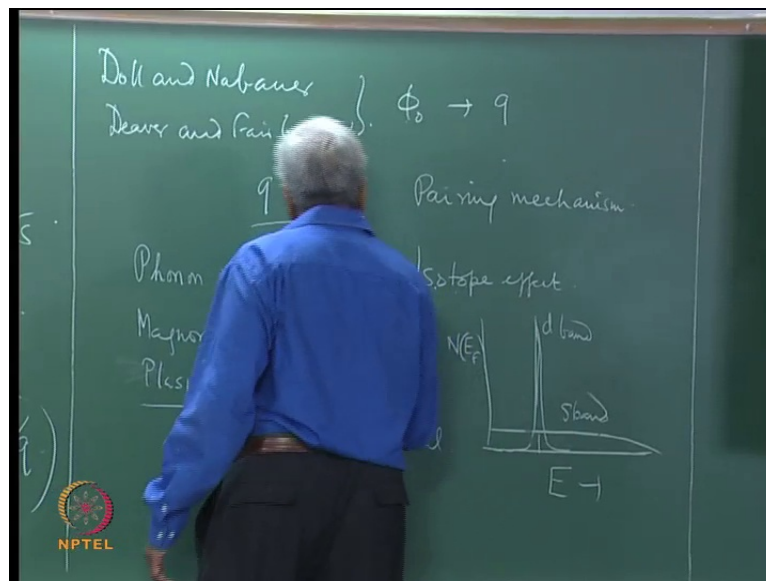


So, we discuss this already also an tunneling of the electrons in the I V characteristics, which shows the onset of current when the biasing of voltage of the tunnel junction exceed that of the energy gap then current starts for ((Refer Time: 06:07)). So, that is again, so these are the various experiments to which we know that there is the energy gap in the excitation spectrum of the electrons, when the material become superconductor. The other important experiment associated, this is flux quantization which we discussed already the quantum mechanical phase of a superconductor goes as e to the power i $\oint (\hbar \nabla \psi - q \vec{A}) \cdot d\vec{l}$ is integral by \hbar cross. So, the or $q \vec{A}$, the q is the charge. So, this is the form of the wave function. So, in order to that this wave function is single valued when there is a magnetic field, where's \vec{A} is a vector potential. So, when we apply a magnetic field, the phase factor is related to the line integral of \vec{A} by stock theorem this becomes

$\oint \nabla \times \mathbf{A} \cdot d\mathbf{s}$, and this is just nothing but B and this is what we call the magnetic flux through the loop.

So, the phase factor goes as q by h cross times ϕ , the ϕ is the magnetic flux. So, this in order to ψ is single valued, when one goes through close loop inside this superconductor, this should be an integral multiple of 2π . In other words ϕ should be h by q times n or $n \phi_0$, where ϕ_0 is the flux quantum, h is flux constant, q is the charge carried by the carriers in the superconductor.

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Now, in the experimental measurement of the flux quantum by Doll and Deaver and Fairbank independently determine the flux quantum, such that q can be evaluated from this. Since h is a constant determination of the flux quantum enables us to know the value of q , and both are found independently the q is twice the electronic charge. And that is a convincing evidence for the existence of Cooper pairs which a pair of electrons carries a charge of twice the electron charge. So, the determination of flux quantum, gave conclusive evidence regarding the pairing mechanism, which is responsible for the superconducting behavior.

So, essentially nowadays if you want to account for the superconducting nature of a material new material, one looks for the pairs, and the immediate question is how does the pairing arise? So, the theory which was discussed first by Cooper is based on the phonon mechanism of pairing. This is also supported by the experimental

observation of the so-called isotropic effect, since this phonon mechanism depends on the vibration of the crystal lattice. So, the harmonic nature means that there is a dependence on the mass for the coupling. So, they found that the transition temperature depends on the mass of the ion involved, so this again indicated at phonon, so somehow involved in bringing about the pairing, but it is not necessary that you should only be the phonon mechanisms anything that which the conduction electrons are coupled, any excitation. For example, magnon are there, exciton are there or plasmon's are there, and so on so. All these can be pass any of these elementary excitation in a crystal lattice, which can couple to the electronic systems can provide parrying mechanisms.

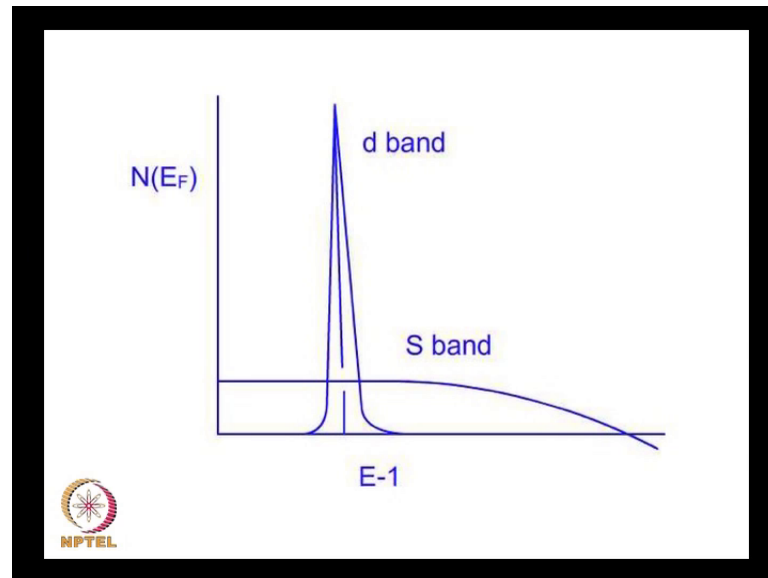
So, it is not necessary should be the phonon mechanisms from the phonon mechanisms is the most obvious and simple is of the possible mechanisms, but other mechanisms cannot also exists what is crucial is there is a pairing of the electrons. So, the formation of the cooper pairs is crucial to be superconducting the feature of any material. and because of the phonon mechanism which indicates that the energy binding energy goes as exponential minus 2 by $n e f v$ this is the three axis for free exponential factor this is only weakly dependent on the free exponential factors, the main temperature dependent's occurrence of the argument the exponent's.

So, they density as state the product of the electronic density of states, and the coupling; this is the crucial factor which decides how much the energy is lower and how strong is the binding between the cooper pairs, and that is also the reason why when we extra large, the electron phonon coupling is strong. Usually we have already discussed the mechanism of electrical resistivity the normal metal, in the presence of a strong phonon electron coupling, the material is going to be a poor conductor having high resistance electrical resistance in the normal stay. And that is also the condition of the occurrence of superconductivity, which is against the experimental fact, that it is usually the poor were conducting metals such as led or aluminum, which becomes superconducting rather than the very good conductors like silver or gold or copper for that metals.

So, this is also experimentally go now. Similarly the electronic density a sate is another crucial factor determining extent of winding of the cooper pairs, and this is again seen experimentally in the sense at most to the superconductors $I T c$ superconductors, which have a high binding energy which indicates high binding energies for cooper pairs are all involving a transition metal. And transition metals because of the D band electrons, so

niobium all these of transition. So, there all here high pick, because of the narrow D band they are strongly peaked at the fermi level and therefore, the electronic density of states at the fermi level tends to be very large.

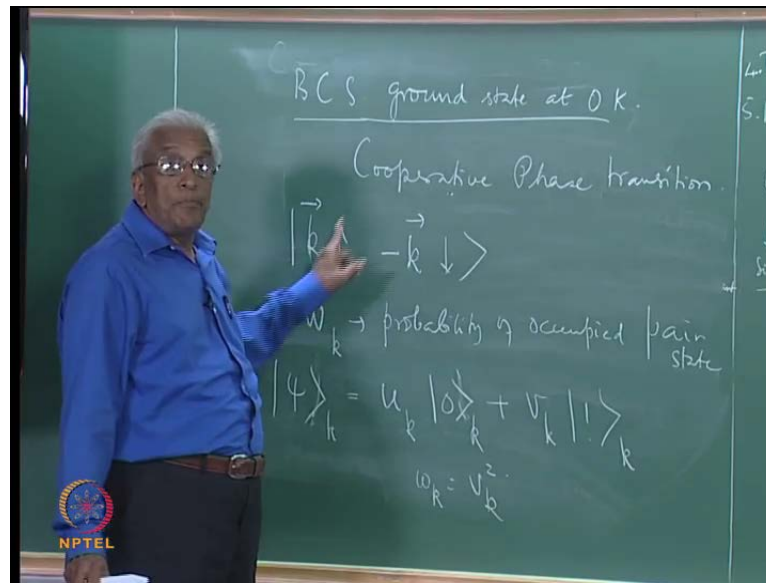
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So, if you see, so these are narrow for example, a conventional metal like this. So, you can see a sharply peak d band metal, this is an s band metal. So, this is the fermi level. So, you can see that a d band metal has a larger density of state, therefore there are more prone to have a higher T_c the transition temperature the conventional s band metal that is also experimentally seen.

So, these are all strong dedication that basic mechanism of being propose padding mechanism as the essentially correct. However, in case of the ground state of BCS superconductors and I have only discussed the formation of a pair by being coupling between the two electrons, but a BCS superconductor consist of a very large number of electrons something like that 23 electron.

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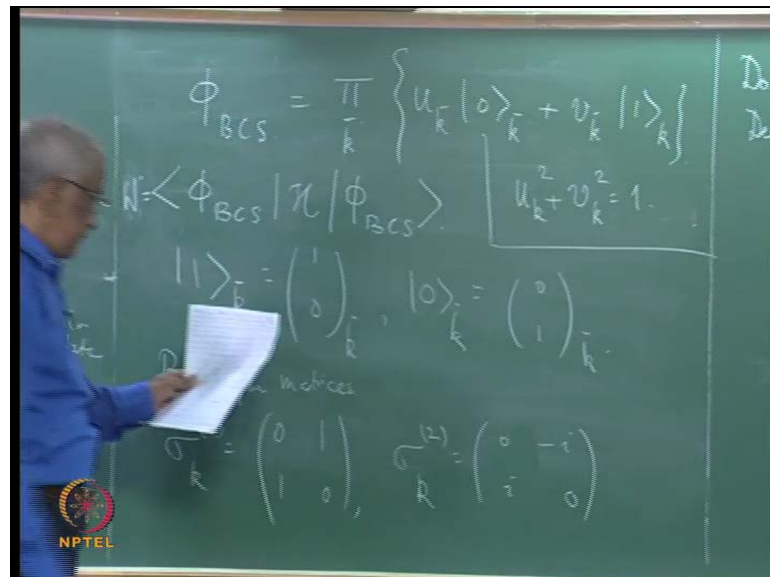
So, we are in order to discuss the energetic of the BCS ground state at 0 kelvin, we have to discuss how all the 24, 23 electrons form pairs, this is and we also know the superconductor transition is a cooperative transition which takes place in a very narrow temperature interval. And this is because when the energies is lower than the formation of cooper pairs, it is energetically favorable this leads to the formation of additional pairs and so this becomes a cooperative phase transition. So, the entire T f conduction electron forms pairs. So, this is the essence of the cooperative phase transition, and we have to talk about how the assembly of large number of electrons forms pairs, this was discussed by BCS and for these we have to discuss the formation of the cooper pairs state, which is characterized by this, the cooper pairs wave function is characterized by this.

So, we have a state in which both states with plus k and minus k with an up stiff spin and a down spin; these two states of the normal electrons are both completely occupied or completely empty. So, the wave functions, if you want to write the probability that a pair state occupied that the state is occupied by a pair of electron. If w_k is the probability, then we have the wave function can be written as $u_k |0\rangle_k + v_k |1\rangle_k$, where w_k just a the square of the v_k , we assume u_k and v_k to be both real for simplicity. And the state $|0\rangle_k$ and $|1\rangle_k$ indicate that the state with the wave vector k is simultaneously occupied by a pair of electrons which momentum k and minus k wave vector k and minus k with up- and down spin. So, then this is called one k. So, it is a state with two electrons occupying such a whereas if it is $|0\rangle_k$; that means this state is completely empty. So, u_k is the

probability that the state is a state with k is completely unoccupied, whereas v_k square is the probability whether it is completely occupied.

So, the states are either occupied together in pairs or completely unoccupied, and v_k square is just the probability of transition where probability of occupation, which is w_k . So, this is the essential we function of these two electrons state paired state with wave vector k . And the BCS wave function of the ground state of a BCS superconductor can be written in the form of a product of such paired states in which the electron, the states are either completely occupied by a pair of electron or both are completely empty.

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So, we write the ϕ_{BCS} the ground state wave function a consist of a product of such states $u_k |0\rangle_k + v_k |1\rangle_k$. So, that is the downstate we function $|1\rangle_k$ and this total BCS state is formed of products of such one such states paired states, which means that it assumes that the pairs are non-interacting. Now in order to find they energy of this ground state we have to write Hamiltonian, and then find this energy that is the Hamiltonian of the electrons. So, this is the energy w , and we minimize this with respect to the variation in the para meters u_k and v_k , we have u_k square plus v_k square equal to 1. So, these are not independently vary if you fixed u_k then v_k gets automatically fix and vice versa, therefore enough to vary with respect to one of; these two para meters in order to do that we represent these states $|1\rangle_k$ $|0\rangle_k$ by matrixes k , and $|0\rangle_k$ is $\begin{pmatrix} 0 \\ 1 \end{pmatrix}_k$. In this case we can use the pauli spin matrixes to calculate the expectation values, what are the

Pauli spin matrices? We have their characteristics $\sigma_k^+ \sigma_k^- = 0$ and $\sigma_k^- \sigma_k^+ = 0$, if we have this combination of these can be used to represent the annihilation and creation of pairs in the following way.

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$$\sigma_k^+ = \frac{1}{2} \left\{ \sigma_k^{(1)} + i \sigma_k^{(2)} \right\}$$

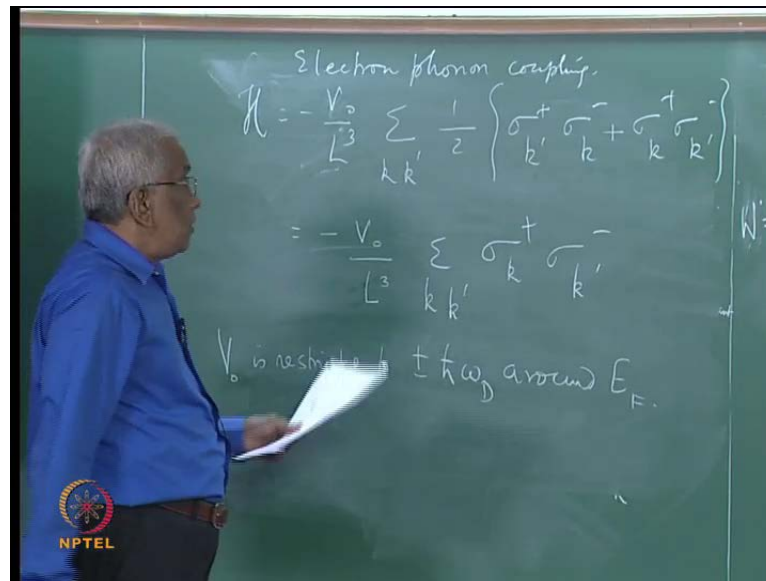
$$\sigma_k^- = \frac{1}{2} \left\{ \sigma_k^{(1)} - i \sigma_k^{(2)} \right\}$$

$$\sigma_k^+ |1\rangle_k = 0, \quad \sigma_k^- |1\rangle_k = |0\rangle_k$$

$$\sigma_k^+ |0\rangle_k = |1\rangle_k, \quad \sigma_k^- |0\rangle_k = 0.$$

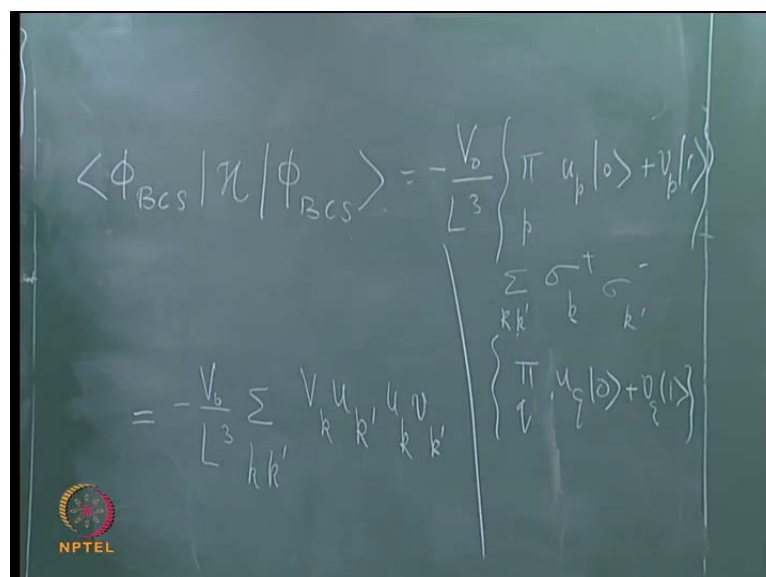
We write σ_k^+ as half of $\sigma_k^{(1)} + i \sigma_k^{(2)}$, and σ_k^- as half of $\sigma_k^{(1)} - i \sigma_k^{(2)}$, in terms of σ_k^+ and σ_k^- . We can show that $\sigma_k^+ \sigma_k^+ = 0$, $\sigma_k^+ \sigma_k^+ = 0$, and $\sigma_k^- \sigma_k^- = 0$, in terms of these we can write the electron-phonon interaction Hamiltonian.

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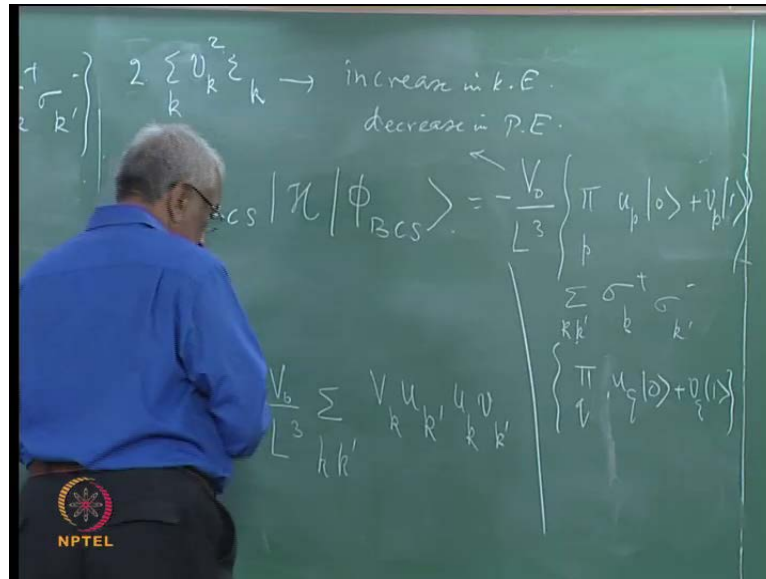
And then find the energy expectation value it turns out that the Hamiltonian, the electron phonon interaction, the Hamiltonian for this turn out to have the form $H = -\frac{V_0}{L^3} \sum_{k, k'} \frac{1}{2} (\sigma_{k'}^+ \sigma_k^- + \sigma_k^+ \sigma_{k'}^-)$, which means that we create an excitation in the state k' , this term where simultaneously removing an excitation. So, this can be written as... So, using this, now V_0 is restricted to plus or minus $\hbar \omega_D$ around Fermi energy, with this we can calculate with this, and the BCS wave function we are now in a position to calculate this in times out.

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That we have the result is equal to minus v naught by L cube pi p u p 0 plus v p 1 times sigma k k prime sigma k plus sigma k prime minus times pi cube u k 0 plus v cube 1. So, we can calculate this using the properties of the Pauli spin matrices, and therefore we have this as minus v naught bi l cube sigma k k prime v k u k prime then u k v k prime. So, we have calculated the net energy value Eigen value of this.

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And we have also the formation of pairs also increasing the kinetic energy by an amount ϵ_k per pair times v_k^2 , which is the probability of the forming pairs. This is because there is a pair. So, that is the increase in kinetic energy is due to pair formation, this is the decreasing in potential energy due to electron-phonon interaction. So, the net BCS energy is a sum of these two and increasing the kinetic energy plus lowering of the potential energy.

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Handwritten equations on a chalkboard:

$$W_{BCS} = 2 \sum_k v_k^2 \xi_k - \frac{V_0}{L^3} \sum_{kk'} v_k u_{k'} / u_k v_{k'}$$

$$\xi_k = \frac{\hbar^2 k^2}{2m} - E_F^0$$

Minimize W_{BCS} w.r.t. v_k/u_k . $v_k^2 + u_k^2 = 1$

$$v_k = \cos \theta_k$$

$$u_k = \sin \theta_k$$

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So, W_{BCS} has some of these two v_k^2 by k minus v_k by $1/L^3$ $\sum_{kk'} v_k u_{k'} / u_k v_{k'}$. Here ξ_k is the kinetic energy of a single electron with respect to the Fermi energy at absolute zero. So, we have to minimize this W_{BCS} with respect to v_k or u_k . So, this is done such that $v_k^2 + u_k^2 = 1$. So, we choose v_k to be $\cos \theta_k$. So, that and u_k to be $\sin \theta_k$. So, this condition is automatically satisfied.

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Handwritten equations on a chalkboard:

$$\frac{\partial W_{BCS}}{\partial \theta_k} = 0$$

$$W_{BCS} = \sum_k 2 \xi_k \cos^2 \theta_k - \frac{V_0}{L^3} \sum_{kk'} \cos \theta_k \sin \theta_{k'} / \cos \theta_{k'} \sin \theta_k$$

$$\frac{\partial W_{BCS}}{\partial \theta_k} = -2 \xi_k \sin 2\theta_k - \frac{V_0}{L^3} \sum_{k'} \cos \theta_{k'} \sin 2\theta_k$$

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So, it is enough if we minimize it rewrite this in terms of the theta k and then minimize it with respect to variation in theta k. So, this is what we will do now. So, we demand that the ground state energy is minimum when D W BCS by D theta k is 0, where W BCS in terms of the theta is $\sum_k \psi_k \cos^2 \theta_k - v_0 \sum_k \cos \theta_k \sin \theta_k$. So, this is what we have to minimize with respect to theta k, and this gives $2 \psi_k \sin 2 \theta_k - v_0 \cos 2 \theta_k = 0$.

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The image shows a chalkboard with the following handwritten equations:

$$\sum_k \tan 2\theta_k = -\frac{1}{2} \frac{V_0}{L^3} \sum_{k'} \sin 2\theta_{k'}$$

$$\Delta = \frac{V_0}{L^3} \sum_{k'} \sin \theta_{k'} \cos \theta_{k'} \rightarrow \text{gap parameter}$$

$$E_k = \sqrt{\sum_k^2 + \Delta^2}$$

$$\tan 2\theta_k = -\frac{\Delta}{\epsilon_k}$$

$$\sin 2\theta_k = \frac{\Delta}{E_k}$$

So, that the condition for minimum this is equal to 0 gives the important result ψ_k , and $2 \theta_k = \arctan(-\frac{v_0 \sum_{k'} \sin \theta_{k'} \cos \theta_{k'}}{\psi_k})$. So, that the essential condition for a minimum of the energy. Now we designate a parameter delta as $\Delta = \frac{v_0}{L^3} \sum_{k'} \sin \theta_{k'} \cos \theta_{k'}$ with that short hand, we have and also be right $E_k = \sqrt{\psi_k^2 + \Delta^2}$, delta is known as the gap parameter. In terms of these this condition reduces to $\tan 2 \theta_k = -\frac{\Delta}{\psi_k}$ which also mean $\sin 2 \theta_k = \frac{\Delta}{E_k}$ where ψ_k is defined by this. So, this is the condition for minimum and we use this to calculate the minimum energy, which is the energy of the ground state of the BCS superconductor at absolute 0.

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$$w_k = v_k^2 = \frac{1}{2} \left(1 - \frac{\psi_k}{E_k} \right)$$

$$= \frac{1}{2} \left(1 - \frac{\psi_k}{\sqrt{\psi_k^2 + \Delta^2}} \right)$$

$$W_{BCS} = \sum_k \psi_k \left(1 - \frac{\psi_k}{E_k} \right) - \frac{L^3}{V_0} \Delta^2$$

$$\text{Normal state energy} = \sum_{|k| < k_F} 2 \psi_k$$

So, we get w_k , this is the probability half of $1 - \psi_k$ by k is equal to half of $1 - \psi_k$ by $\psi_k^2 + \Delta^2$ to the power half. So, the w_{BCS} with this minimization turns out to be... So, this is the energy of the energy of the BCS superconducting state at absolute 0, and if he wish to determine whether the superconducting state as the lower energy than the normal state. We have to subtract this energy from the normal state energy, which is $\sum_{|k| < k_F} 2 \psi_k$ where these fermi wave vector of 2. So, if we remove this energy if we find the difference between these two, and if it is negative; that means that the BCS superconducting state is energetically lower. And therefore, it is favorable to for the electrons to be compared and form a superconducting state at absolute 0, we will consider this to determine the condensation energy of a superconductor in the next lecture.